

10518612

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 09:21:14 ON 11 JUN 2007

=> FILE REG

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.21	0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 09:21:41 ON 11 JUN 2007

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 JUN 2007 HIGHEST RN 936909-28-3

DICTIONARY FILE UPDATES: 10 JUN 2007 HIGHEST RN 936909-28-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

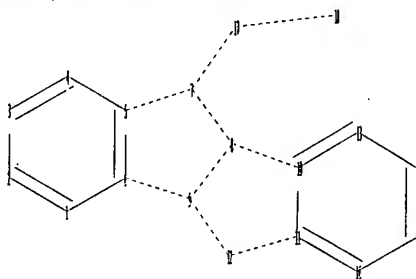
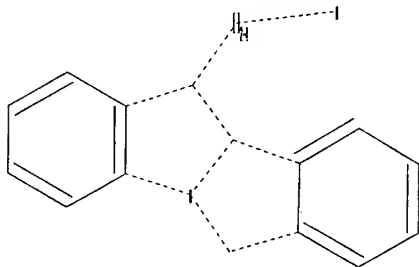
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10518612.str



11/06/2007

10518612

chain nodes :
17 18
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
chain bonds :
7-17 17-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 8-10 9-12 10-11 10-13 11-12
11-16 13-14 14-15 15-16
exact/norm bonds :
5-7 6-9 7-8 7-17 8-9 8-10 9-12 11-12 17-18
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-13 11-16 13-14 14-15 15-16

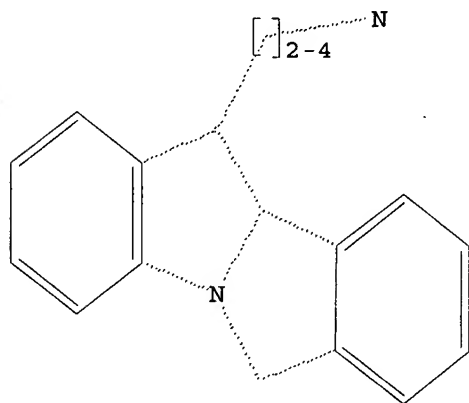
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS

L1 STRUCTURE UPLOADED

=> D

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> S L1

SAMPLE SEARCH INITIATED 09:22:14 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 120 TO ITERATE

100.0% PROCESSED 120 ITERATIONS
SEARCH TIME: 00.00.01

5 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 1743 TO 3057
PROJECTED ANSWERS: 5 TO 234

11/06/2007

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L2 5 SEA SSS SAM L1

=> S L1 FULL

FULL SEARCH INITIATED 09:22:20 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 2433 TO ITERATE

100.0% PROCESSED 2433 ITERATIONS

106 ANSWERS

SEARCH TIME: 00.00.01

L3 106 SEA SSS FUL L1

=> FILE CAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

172.10

172.31

FILE 'CAPLUS' ENTERED AT 09:22:26 ON 11 JUN 2007

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FILE COVERS 1907 - 11 Jun 2007 VOL 146 ISS 25

FILE LAST UPDATED: 10 Jun 2007 (20070610/ED)

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=> S L3

L4 12 L3

=> D IBIB ABS HITSTR TOT

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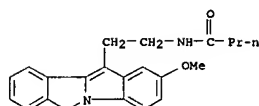
10518612

L4 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2006:1177614 CAPLUS
 DOCUMENT NUMBER: 146:55814
 TITLE: Differences in binding sites of two melatonin receptors help to explain their selectivity to some melatonin analogs: a molecular modeling study
 AUTHOR(S): Chugunov, Anton O.; Farce, Amaury; Chavatte, Philippe;
 CORPORATE SOURCE: Efremov, Roman G. Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences, GSP Moscow, 117997, Russia
 SOURCE: Journal of Biomolecular Structure and Dynamics 24(2), 91-107
 (2006), CODEN: JBSDD6; ISSN: 0739-1102
 PUBLISHER: Adenine Press
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Numerous diseases have been linked to the malfunction of G-protein coupled receptors (GPCRs). Their adequate treatment requires rational design of new high-affinity and high-selectivity drugs targeting these receptors. The authors report three-dimensional models of the human MT1 and MT2 melatonin receptors, members of the GPCR family. The models are based on the x-ray structure of bovine rhodopsin. The computational approach employs an original procedure for optimization of receptor-ligand structures. It includes rotation of one of the transmembrane α -helices around its axis with simultaneous assessment of quality of the resulting complexes according to a number of criteria the authors have developed for this purpose. The optimal geometry of the receptor-ligand binding is selected based on the anal. of complementarity of hydrophobic/hydrophilic properties between the ligand and its protein environment in the binding site. The elaborated "optimized" models are employed to explore the details of protein-ligand interactions for melatonin and a number of its analogs with known affinity to MT1 and MT2 receptors. The models permit rationalization of exptl. data, including those that were not used in model building. The perspectives opened by the constructed models and by the optimization procedure in the design of new drugs are discussed.
 IT 244160-10-9
 RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
 (Three-dimensional models of human melatonin receptors MT1 and MT2 in relation to interactions with melatonin and analogs)
 RN 244160-10-9 CAPLUS
 CN Butanamide, N-[2-(2-methoxy-6H-indololo[2,1-a]indol-11-yl)ethyl]- (CA INDEX NAME)

L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:2887 CAPLUS
 DOCUMENT NUMBER: 140:77024
 TITLE: Preparation of tetracyclic arylalkyl indoles having serotonin receptor affinity
 INVENTOR(S): Jasti, Venkateswarlu; Ramakrishna, Venkata Satya Nirogi; Kambhampati, Rama Sastri; Battula, Srinivasa Reddy; Rao, Venkata Satya Veerabhadra Vadamudi
 PATENT ASSIGNEE(S): Suven Pharmaceuticals Ltd., India
 SOURCE: PCT Int. Appl., 66 pp.
 CODEN: PIXX2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

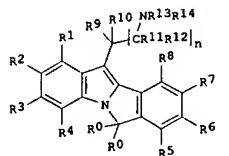
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 200400845	A1	20031231	WO 2003-IN224	20030619
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, JP, KE, KG, KP, KR, KZ, LC, LK, LA, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CH, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
IN 2002MA00476	A	20070518	IN 2002-MA476	20020621
CA 2490115	A1	20031231	CA 2003-2490115	20030619
AU 2003249584	A1	20040106	AU 2003-249584	20030619
BR 2003012175	A	20050405	BR 2003-12175	20030619
EP 1537113	A1	20050608	EP 2003-760859	20030619
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1662538	A	20050831	CN 2003-814597	20030619
JP 2006501175	T	20060112	JP 2004-515420	20030619
US 2005203103	A1	20050915	US 2005-518624	20050513
PRIORITY APPLN. INFO.:			IN 2002-MA476	A 20020621
			WO 2003-IN224	W 20030619
OTHER SOURCE(S):		MARPAT 140:77024		
GI				

L4 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

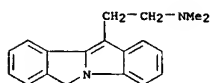


AB The title compds. [I: R0 = H, alkyl; R1-R12 = H, halo, oxo, thio, etc.; or
 or the adjacent groups like R1 and R2, etc. together with carbon atoms to which they are attached may form 5-7 membered ring which may further contain one or more double bonds and/or one or more heteroatoms such as O, N, S or Se; or R9 and R10 or R11 and R12 together with the carbon atoms to which they are attached may form a 3-6 membered ring which may further contain one or more double bonds and/or one or more heteroatoms such as O, N, S or Se; R13 and R14 = H, alkyl, cycloalkyl, aryl, etc.; or NR13R14 = 3-7 membered heterocyclyl; n = 1-8], useful for treating conditions where a modulation of 5-HT and/or serotonin activity is desired (no data), were prepared Thus, reacting 1-(2'-bromobenzyl)-N,N-dimethyltryptamine with N,N-dimethylacetamide in the presence of PdCl2(P(o-tolyl)3)2 and AcOK afforded 11-(2-N,N-dimethylaminoethyl)-6H-indololo[2,1-a]indole. This invention also relates to processes for preparing the compds. I, compns. containing effective amts. of the compound I and the use of such a compound/composition in therapy.
 IT 639808-61-0P 639808-62-1P 639808-63-2P
 639808-64-3P 639808-65-4P 639808-66-5P
 639808-67-6P 639808-68-7P 639808-69-8P
 639808-70-1P 639808-71-2P 639808-72-3P
 639808-73-4P 639808-74-5P 639808-75-6P
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 639809-38-4P 639809-39-5P 639809-41-9P
 639809-42-0P 639809-44-2P 639809-46-4P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of isoindolo[2,1-a]indoles having serotonin receptor affinity)
 RN 639808-61-0 CAPLUS
 CN 6H-isoindolo[2,1-a]indole-11-ethanamine, N,N-dimethyl- (9CI) (CA INDEX NAME)

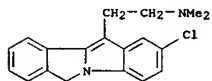
11/06/2007

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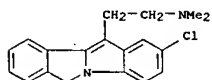
L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 639808-62-1 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-chloro-N,N-dimethyl- (9CI)
 (CA INDEX NAME)



RN 639808-63-2 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-chloro-N,N-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)



• x HCl

RN 639808-64-3 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-chloro-N,N-dimethyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

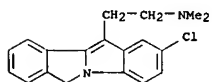
CM 1

CRN 639808-62-1
 CMF C19 H19 Cl N2

L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 ethanedioate (9CI) (CA INDEX NAME)

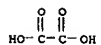
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CRN 639808-62-1
 CMF C19 H19 Cl N2



CM 2

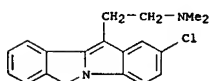
CRN 144-62-7
 CMF C2 H2 O4



RN 639808-67-6 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-chloro-N,N-dimethyl-, 2-hydroxy-1,2,3-propanetricarboxylate (9CI) (CA INDEX NAME)

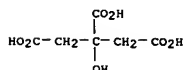
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CRN 639808-62-1
 CMF C19 H19 Cl N2

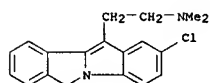


CM 2

CRN 77-92-9
 CMF C6 H8 O7



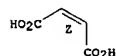
L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 110-16-7
 CMF C4 H4 O4

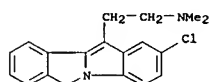
Double bond geometry as shown.



RN 639808-65-4 CAPLUS
 CN Butanedioic acid, hydroxy-, compd. with 2-chloro-N,N-dimethyl-6H-isoindolo[2,1-a]indole-11-ethanamine (9CI) (CA INDEX NAME)

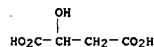
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CM 2

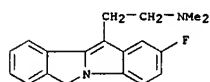
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 CMF C4 H6 O5



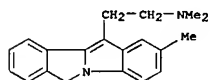
RN 639808-66-5 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-chloro-N,N-dimethyl-,

L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

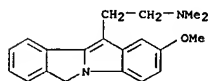
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 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-fluoro-N,N-dimethyl- (9CI)
 (CA INDEX NAME)



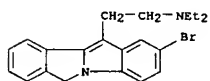
RN 639808-69-8 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, N,N,2-trimethyl- (9CI) (CA INDEX NAME)



RN 639808-70-1 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-methoxy-N,N-dimethyl- (9CI)
 (CA INDEX NAME)



RN 639808-71-2 CAPLUS
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-bromo-N,N-diethyl- (9CI) (CA INDEX NAME)

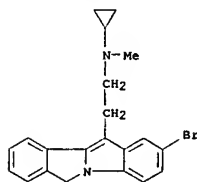


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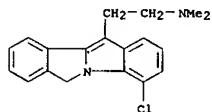
11/06/2007

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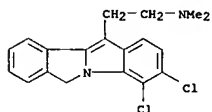
L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 639808-73-4 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 4-chloro-N,N-dimethyl- (9CI)
(CA INDEX NAME)

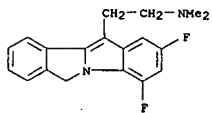


RN 639808-74-5 CAPLUS
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(CA INDEX NAME)

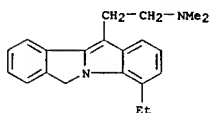


RN 639808-75-6 CAPLUS
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(CA INDEX NAME)

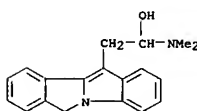
L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



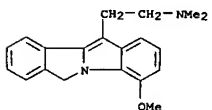
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CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 4-ethyl-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 639808-86-9 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanol, alpha-(dimethylamino)- (9CI) (CA INDEX NAME)



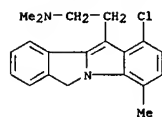
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(CA INDEX NAME)



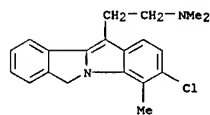
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11/06/2007

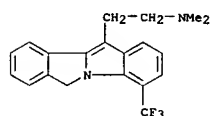
L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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(CA INDEX NAME)

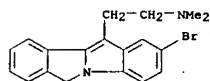


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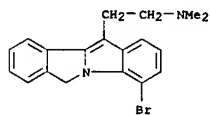


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(CA INDEX NAME)

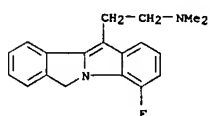
L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 639808-89-2 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 4-bromo-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 639808-90-5 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 4-fluoro-N,N-dimethyl- (9CI)
(CA INDEX NAME)



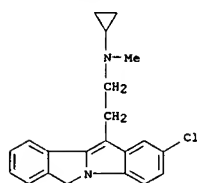
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CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-chloro-N-cyclopropyl-N-methyl-, 2-hydroxy-1,2,3-propanetricarboxylate (9CI) (CA INDEX NAME)

CN 1

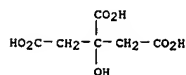
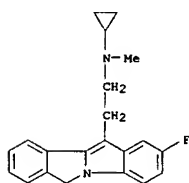
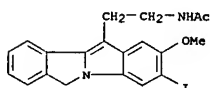
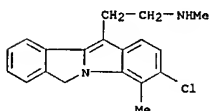
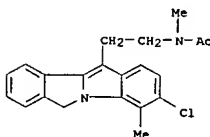
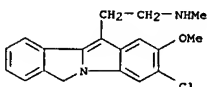
CRN 639809-22-6
CMF C21 H21 Cl N2

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L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



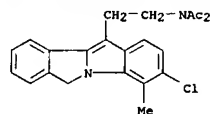
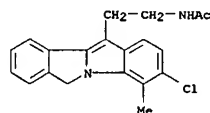
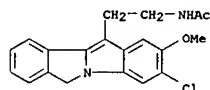
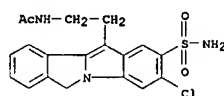
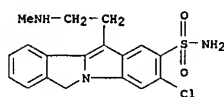
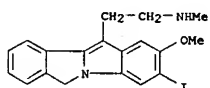
CM 2

CRN 77-92-9
CMF C6 H8 O7RN 639809-25-9 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, N-cyclopropyl-2-fluoro-N-methyl- (9CI) (CA INDEX NAME)RN 639809-27-1 CAPLUS
CN Acetamide, N-[2-(3-chloro-4-methyl-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(9CI) (CA INDEX NAME)RN 639809-39-5 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3-chloro-N,4-dimethyl- (9CI)
(CA INDEX NAME)RN 639809-41-9 CAPLUS
CN Acetamide, N-[2-(3-chloro-4-methyl-6H-isoindolo[2,1-a]indol-11-yl)ethyl]-N-methyl- (9CI) (CA INDEX NAME)RN 639809-42-0 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3-chloro-2-methoxy-N-methyl- (9CI) (CA INDEX NAME)

RN 639809-44-2 CAPLUS

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L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 639809-29-3 CAPLUS
CN Acetamide, N-[2-(3-chloro-4-methyl-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)RN 639809-32-8 CAPLUS
CN Acetamide, N-[2-(3-chloro-2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)RN 639809-35-1 CAPLUS
CN Acetamide, N-[2-(2-(aminosulfonyl)-3-chloro-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)RN 639809-38-4 CAPLUS
CN Acetamide, N-[2-(3-iodo-2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 6H-Isoindolo[2,1-a]indole-2-sulfonamide, 3-chloro-11-[2-(methylamino)ethyl]- (9CI) (CA INDEX NAME)RN 639809-46-4 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3-iodo-2-methoxy-N-methyl- (9CI)
(CA INDEX NAME)REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

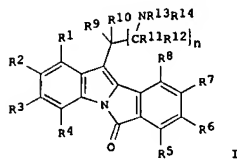
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L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:2617 CAPLUS
 DOCUMENT NUMBER: 140:77023
 TITLE: Preparation of novel tetracyclic arylcarbonyl indoles having serotonin receptor affinity
 INVENTOR(S): Jasti, Venkateswarlu; Ramakrishna, Venkata Satya Nirogi; Kambhampati, Rama Sastri; Battula, Srinivasa Reddy; Rao, Venkata Satya Veerabhadra Vadiamudi
 PATENT ASSIGNEE(S): Suven Pharmaceuticals Ltd., India; Suven Life Sciences
 SOURCE: PCT Int. Appl., 63 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004000205	A2	20031231	WO 2003-IN223	20030619
WO 2004000205	A3	20040408		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
IN 2002MA00477	A	20060915	IN 2002-MA477	20020621
CA 2490002	A1	20031231	CA 2003-2490002	20030619
AU 2003249583	A1	20040106	AU 2003-249583	20030619
EP 1517909	A2	20050330	EP 2003-760858	20030619
EP 1517909	B1	20061025		
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AT 343580	T	20061115	AT 2003-760858	20030619
US 2005250834	A1	20051110	US 2005-518612	20050513
HK 1074630	A1	20070119	HK 2005-108744	20050930
PRIORITY APPLN. INFO.:			IN 2002-MA477	A 20020621
			WO 2003-IN223	W 20030619

OTHER SOURCE(S): MARPAT 140:77023
 GI

L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB The title compds. [I; R1-R12 = H, halo, oxo, thio, etc.; or the adjacent groups like R1 and R2, etc. together with carbon atoms to which they are attached may form 3-7 membered ring which may further contain one or more double bonds and/or one or more heteroatoms such as O, N, S or Se; or R9 and R10 or R11 and R12 together with the carbon atoms to which they are attached may form a 3-6 membered ring which may further contain one or more double bonds and/or one or more heteroatoms such as O, N, S or Se; R13 and R14 = H, alkyl, cycloalkyl, aryl, etc.; or NR13R14 = 3-7 membered heterocyclyl; n = 1-8], useful for treating conditions where a modulation of 5-HT and/or serotonin activity is desired (no data), were prepared

Thus, reacting 1-(2'-bromobenzoyl)-N,N-dimethyltryptamine with N,N-dimethylacetamide in the presence of PdCl2(P(o-tolyl)3)2 and AcOK afforded 11-(2-N,N-dimethylaminoethyl)-6H-isoindolo[2,1-a]indol-6-one. This invention also relates to processes for preparing the compds. I, compns.

containing effective amts. of the compound I and the use of such a compound/composition in therapy.

IT 639805-04-2P 639805-05-3P 639805-06-4P
 639805-07-5P 639805-08-6P 639805-09-7P
 639805-10-0P 639805-11-1P 639805-12-2P
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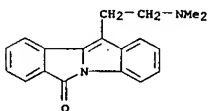
RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of isoindolo[2,1-a]indolones having serotonin receptor affinity)

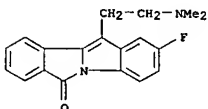
RN 639805-04-2 CAPLUS

CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)

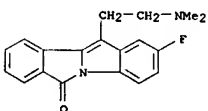
L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 639805-05-3 CAPLUS
 CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro- (9CI) (CA INDEX NAME)



RN 639805-06-4 CAPLUS
 CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro-, monohydrochloride (9CI) (CA INDEX NAME)



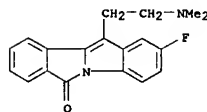
• HCl

RN 639805-07-5 CAPLUS
 CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 639805-05-3
 CMF C19 H17 F N2 O

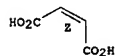
L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 110-16-7
 CMF C4 H4 O4

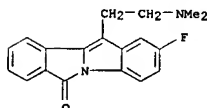
Double bond geometry as shown.



RN 639805-08-6 CAPLUS
 CN Butanedioic acid, hydroxy-, compd. with 11-[2-(dimethylamino)ethyl]-2-fluoro-6H-isoindolo[2,1-a]indol-6-one (9CI) (CA INDEX NAME)

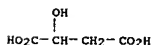
CM 1

CRN 639805-05-3
 CMF C19 H17 F N2 O



CM 2

CRN 6915-15-7
 CMF C4 H6 O5



RN 639805-09-7 CAPLUS
 CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro-,

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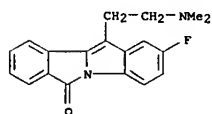
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L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 639805-05-3

CMF C19 H17 F N2 O



CM 2

CRN 144-62-7

CMF C2 H2 O4



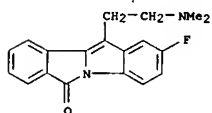
RN 639805-10-0 CAPLUS

CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro-2-hydroxy-1,2,3-propanetricarboxylate (9CI) (CA INDEX NAME)

CM 1

CRN 639805-05-3

CMF C19 H17 F N2 O



CM 2

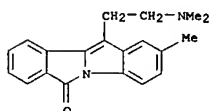
CRN 77-92-9

CMF C6 H8 O7

L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

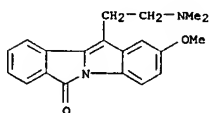
RN 639805-14-4 CAPLUS

CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-methyl- (9CI) (CA INDEX NAME)



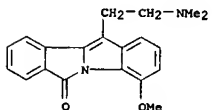
RN 639805-15-5 CAPLUS

CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-methoxy- (9CI) (CA INDEX NAME)



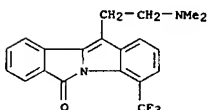
RN 639805-16-6 CAPLUS

CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-4-methoxy- (9CI) (CA INDEX NAME)

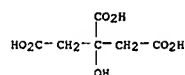


RN 639805-17-7 CAPLUS

CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

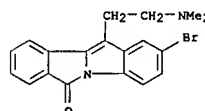


L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



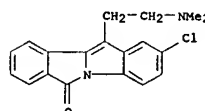
RN 639805-11-1 CAPLUS

CN 6H-Isoindolo[2,1-a]indol-6-one, 2-bromo-11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)



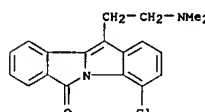
RN 639805-12-2 CAPLUS

CN 6H-Isoindolo[2,1-a]indol-6-one, 2-chloro-11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)



RN 639805-13-3 CAPLUS

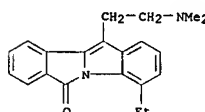
CN 6H-Isoindolo[2,1-a]indol-6-one, 4-chloro-11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

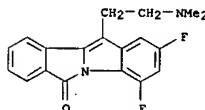
RN 639805-18-8 CAPLUS

CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-4-ethyl- (9CI) (CA INDEX NAME)



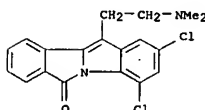
RN 639805-19-9 CAPLUS

CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2,4-difluoro- (9CI) (CA INDEX NAME)



RN 639805-20-2 CAPLUS

CN 6H-Isoindolo[2,1-a]indol-6-one, 2,4-dichloro-11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)



RN 639805-21-3 CAPLUS

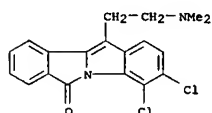
CN 6H-Isoindolo[2,1-a]indol-6-one, 3,4-dichloro-11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)



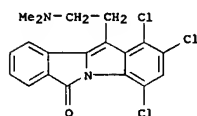
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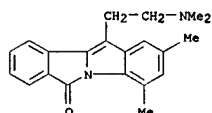
L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



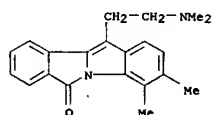
RN 639805-22-4 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 1,2,4-trichloro-11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)



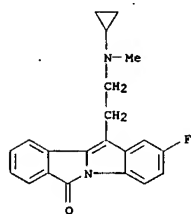
RN 639805-24-6 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2,4-dimethyl- (9CI) (CA INDEX NAME)



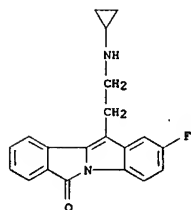
RN 639805-25-7 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-3,4-dimethyl- (9CI) (CA INDEX NAME)



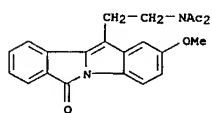
L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 639805-52-0 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(cyclopropylamino)ethyl]-2-fluoro- (9CI) (CA INDEX NAME)



RN 639805-53-1 CAPLUS
CN Acetamide, N-[2-(2-methoxy-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

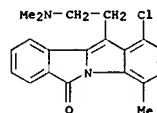


RN 639805-54-2 CAPLUS
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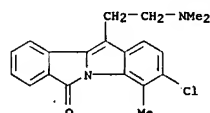
11/06/2007

L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

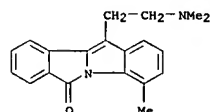
RN 639805-26-8 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 1-chloro-11-[2-(dimethylamino)ethyl]-4-methyl- (9CI) (CA INDEX NAME)



RN 639805-27-9 CAPLUS
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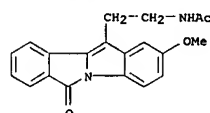


RN 639805-28-0 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-4-methyl- (9CI) (CA INDEX NAME)

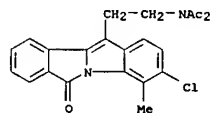


RN 639805-51-9 CAPLUS
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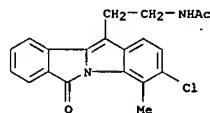
L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



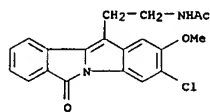
RN 639805-55-3 CAPLUS
CN Acetamide, N-[2-(3-chloro-4-methyl-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 639805-56-4 CAPLUS
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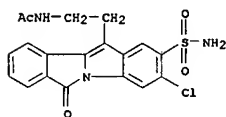
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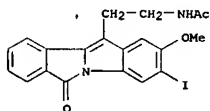
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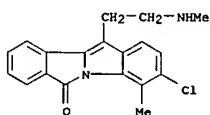
L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
11-yl]ethyl]- (9CI) (CA INDEX NAME)



RN 639805-59-7 CAPLUS
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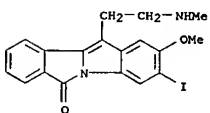


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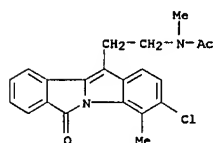


RN 639805-61-1 CAPLUS
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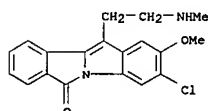
L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



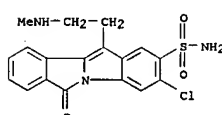
L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 639805-62-2 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 3-chloro-2-methoxy-11-[2-(methylamino)ethyl]- (9CI) (CA INDEX NAME)



RN 639805-63-3 CAPLUS
CN 6H-Isoindolo[2,1-a]indole-2-sulfonamide, 3-chloro-11-[2-(methylamino)ethyl]-6-oxo- (9CI) (CA INDEX NAME)



RN 639805-64-4 CAPLUS
CN 6H-Isoindolo[2,1-a]indol-6-one, 3-iodo-2-methoxy-11-[2-(methylamino)ethyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:215250 CAPLUS
DOCUMENT NUMBER: 138:362155
TITLE: Three-Dimensional Quantitative Structure-Activity Relationship Studies on Selected MT1 and MT2

Melatonin Receptor Ligands: Requirements for Subtype

and Intrinsic Activity Modulation
AUTHOR(S): Rivara, Silvia; Mor, Marco; Silva, Claudia; Zulliani, Valentina; Vaccondio, Federica; Spadoni, Gilberto; Bedini, Annalisa; Tazzia, Giorgio; Lucini, Valeria; Pannacchi, Marilou; Frascchini, Franco; Plazzi, Pier Vincenzo

CORPORATE SOURCE: Dipartimento Farmaceutico, Università degli Studi di Parma, Parma, I-43100, Italy
SOURCE: Journal of Medicinal Chemistry (2003), 46(8), 1429-1439

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The three-dimensional quant. structure-activity relation comparative mol. field anal. (3D-QSAR CoMFA) approach was applied to some classes of melatonin (MLT) membrane receptor ligands, with the principal aim of exploring the correlation between their steric features and MT2-selective antagonism. Binding data obtained from cloned MT1 and MT2 receptor subtypes were used to develop 3D-QSAR models for agonists and for antagonists at the two receptor subtypes, looking for the structural requirements for receptor subtype selectivity. In particular, we superposed the compds. showing antagonist activity, or very low intrinsic activity at the GTPyS test, following the hypothesis that the occupation of an addnl. pocket positioned out of the plane of MLT is one of the major determinants for MT2 selectivity; the statistical models obtained confirmed this hypothesis. Structure-intrinsic activity relation studies, applied to a set of compds. homogeneously tested, allowed the identification of the structural features whose modulation shifts the behavior from that of the agonist to that of the antagonist. The pocket out of the plane of MLT was identified as one of the key features for obtaining selective MT2 antagonists. The reliability of our statistical models was further confirmed by the correct prediction of the pharmacol. behavior of some N-substituted melatonin derivs., which were prepared and tested on cloned receptor subtypes.

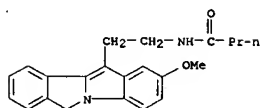
IT 244160-10-9 263865-08-3 263865-09-4
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263865-17-4 263865-18-5 263865-19-6
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR of MT1 and MT2 melatonin receptor ligands)

RN 244160-10-9 CAPLUS
CN Butanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (CA INDEX NAME)

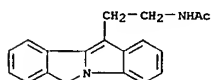
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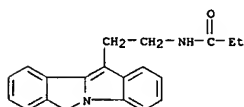
L4 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263865-08-3 CAPLUS
CN Acetamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

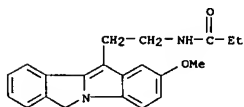


RN 263865-09-4 CAPLUS
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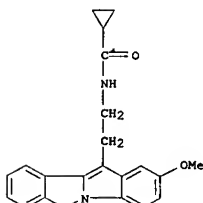


RN 263865-11-8 CAPLUS
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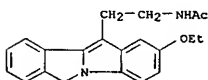
L4 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263865-15-2 CAPLUS
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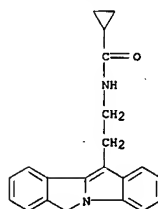


RN 263865-16-3 CAPLUS
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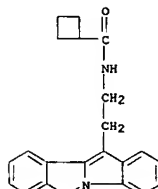


RN 263865-17-4 CAPLUS
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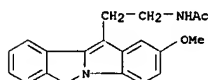
L4 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263865-12-9 CAPLUS
CN Cyclobutanecarboxamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

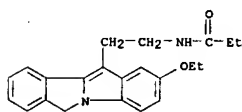


RN 263865-13-0 CAPLUS
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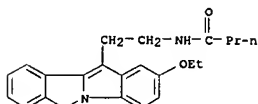


RN 263865-14-1 CAPLUS
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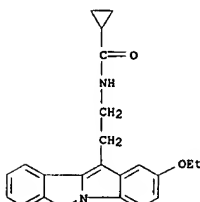
L4 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263865-18-5 CAPLUS
CN Butanamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 263865-19-6 CAPLUS
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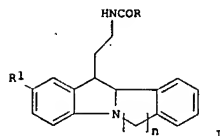


REFERENCE COUNT: 69
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

11/06/2007

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L4 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2002:974419 CAPLUS
 DOCUMENT NUMBER: 138:395420
 TITLE: 3D-QSAR analyses of melatonin antagonists
 AUTHOR(S): Zhu, Li-Li; Xu, Xiao-Jie
 CORPORATE SOURCE: College Chem. Molecular Eng., Peking Univ., Beijing, 100871, Peop. Rep. China
 SOURCE: Wuli Huaxue Xuebao (2002), 18(12), 1087-1092
 CODEN: WHXUEU; ISSN: 1000-6818
 PUBLISHER: Beijing Daxue Chubanshe
 DOCUMENT TYPE: Journal
 LANGUAGE: Chinese
 GI



AB In this paper, two kinds of 3D-QSAR techniques: comparative mol. fields anal. (ComFA) and comparative similarity indexes anal. (ComSIA) were applied using a data set of 37 melatonin antagonists (I, R=alkyl or alicyclyl; R1=H, Cl, or alkoxy; n=1-3). The influences of different grid spacing and partial charge models were systematically investigated. The ComFA contour plots identified several essential features including

steric and electrostatic fields, which are valuable for us to take insight into the mechanisms of the intermol. interactions between inhibitors and receptor.

IT 532394-07-3 532394-08-4 532394-09-5

532394-10-8 532394-12-0 532394-13-1

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532394-18-6 532394-20-0 532394-21-1

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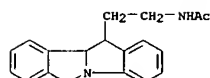
RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)

(3D-QSAR analyses of melatonin antagonists)

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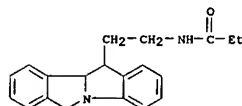
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L4 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



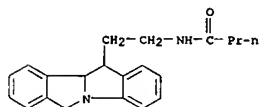
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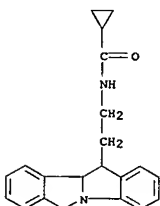
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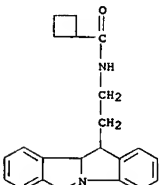
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L4 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



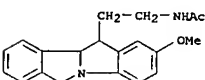
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CN Cyclobutanecarboxamide, N-[2-(10b,11-dihydro-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



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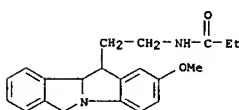
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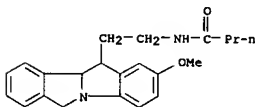
CN Propanamide, N-[2-(10b,11-dihydro-2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



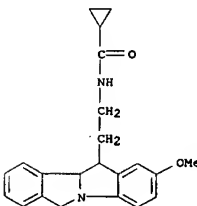
RN 532394-15-3 CAPLUS

CN Butanamide, N-[2-(10b,11-dihydro-2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 532394-16-4 CAPLUS

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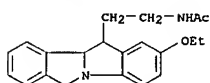
RN 532394-18-6 CAPLUS

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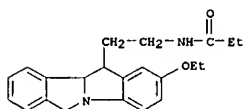
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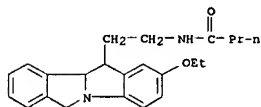
L4 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 532394-20-0 CAPLUS
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RN 532394-21-1 CAPLUS
CN Butanamide, N-[2-(2-ethoxy-10b,11-dihydro-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 532394-22-2 CAPLUS
CN Cyclopropanecarboxamide, N-[2-(2-ethoxy-10b,11-dihydro-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

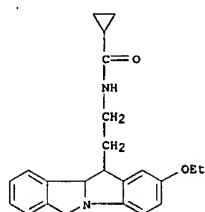
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DOCUMENT NUMBER: 136:64149
TITLE: 6H-isoindolo[2,1-a]indoles or 5,6-dihydroindolo[2,1-a]isoquinolines as subtype-selective melatonergics for therapeutic use
INVENTOR(S): Jones, Robert M.
PATENT ASSIGNEE(S): Cognetix, Inc., USA
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002000215	A1	20020103	WO 2001-US19958	20010622
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TN				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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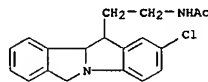
OTHER SOURCE(S): MARPAT 136:64149
AB The invention discloses the use of MT2 selective melatonergics as anticonvulsant agents and as analgesic agents. More specifically, the invention discloses the use of 6H-isoindolo[2,1-a]indoles or 5,6-dihydroindolo[2,1-a]isoquinolines which have melatonin agonist activity and which are selective for the MT2 receptor as anticonvulsant agents or analgesic agents. The invention further relates to the use of 5,6-dihydroindolo[2,1-a]isoquinolines and 6,7-dihydro-5H-benzo[c]azepino[2,1-a]indoles which have melatonin antagonist activity and which are selective for the MT2 receptor as pharmacol. tools for delineation of physiol. responses governed by MT2 receptor activation either by melatonin or selective agonists disclosed herein and for treatment of disorders associated with overprod. of melatonin such as seasonal affective disorder (SAD) and shift work syndrome. Such melatonin

antagonists are also useful for treating Parkinson's Disease.
IT 263865-14-1, CGX 031-120
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(isoindoloindole derivs. and dihydroindoloisoquinoline derivs. as subtype-selective melatonergics for therapeutic use)
RN 263865-14-1 CAPLUS
CN Propanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

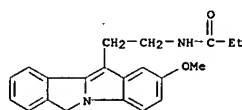
L4 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



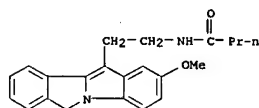
RN 532394-24-4 CAPLUS
CN Acetamide, N-[2-(2-chloro-10b,11-dihydro-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



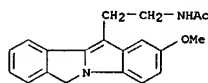
L4 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 244160-10-9, CGX 031139 263865-13-0, CGX 031133
RL: BSU (Biological study, unclassified); BIOL (Biological study) (phenylindole-like behavior; isoindoloindole derivs. and dihydroindoloisoquinoline derivs. as subtype-selective melatonergics for therapeutic use)
RN 244160-10-9 CAPLUS
CN Butanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (CA INDEX NAME)



RN 263865-13-0 CAPLUS
CN Acetamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

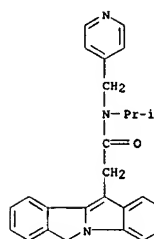
11/06/2007

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L4 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:246308 CAPLUS
 DOCUMENT NUMBER: 135:70637
 TITLE: 2-Arylindole-3-acetamides FPP-Competitive inhibitors of farnesyl protein transferase
 AUTHOR(S): Trotter, B. W.; Quigley, A. G.; Lumma, W. C.; Sisko, J. T.; Walsh, E. S.; Hamann, C. S.; Robinson, R. G.; Bhinnathwala, H.; Kolodin, D. G.; Zheng, W.; Buser, C.
 CORPORATE SOURCE: A.; Huber, H. E.; Lobell, R. B.; Kohl, N. E.; Williams, T. M.; Graham, S. L.; Dinsmore, C. J. Department of Medicinal Chemistry, Merck Research Laboratories, West Point, PA, 19486, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(7), 865-869
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A series of 2-arylindole-3-acetamide farnesyl protein transferase inhibitors has been identified. The compds. inhibit the enzyme in a farnesyl pyrophosphate-competitive manner and are selective for farnesyl protein transferase over the related enzyme geranylgeranyltransferase-I.
 A representative member of this series of inhibitors demonstrates equal effectiveness against HDJ-2 and K-Ras farnesylation in a cell-based assay when geranylgeranylation is suppressed.
 IT 347373-82-4P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 of (arylindole acetamides farnesyl pyrophosphate-competitive inhibitors of farnesyl protein transferase)
 RN 347373-82-4 CAPLUS
 CN 6H-isoindolo[2,1-a]indole-11-acetamide, N-(1-methylethyl)-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



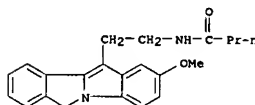
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
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L4 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

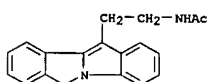
ACCESSION NUMBER: 2000:185117 CAPLUS
 DOCUMENT NUMBER: 132:27842
 TITLE: Mapping the Melatonin Receptor. 6. Melatonin Agonists and Antagonists Derived from 6H-isoindolo[2,1-a]indoles, 5,6-dihydroindolo[2,1-a]isoquinolines, and 6,7-dihydro-5H-benzo[c]azepino[2,1-a]indoles
 AUTHOR(S): Faust, Ruediger; Garratt, Peter J.; Jones, Rob; Yeh, Li-Kuan; Tsotinis, Andrew; Panoussopoulou, Maria; Calogecopoulou, Theodora; Teh, Muy-Teck; Sugden, David
 CORPORATE SOURCE: Department of Chemistry, University College London, London, WC1H 0AJ, UK
 SOURCE: Journal of Medicinal Chemistry (2000), 43(6), 1050-1061
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB 6H-isoindolo[2,1-a]indoles, 5,6-dihydroindolo[2,1-a]isoquinolines, and 6,7-dihydro-5H-benzo[c]azepino[2,1-a]indoles have been prepared as melatonin analogs to investigate the nature of the binding site of the melatonin receptor. The affinity of analogs was determined in a radioligand binding assay using cloned human mtl and MT2 receptor subtypes expressed in NIH 3T3 cells. Agonist and antagonist potency was measured using the pigment aggregation response of a clonal line of Xenopus laevis melanophores.
 The 2-methoxyisoindolo[2,1-a]indoles showed much higher binding affinities than the parent isoindoles and whereas 2-methoxyisoindolo[2,1-a]indoles were agonists in the functional assay, its cyclopropanecarbonyl derivative and parent isoindoles were antagonists. The 2-ethoxyisoindolo[2,1-a]indoles showed reduced binding affinities compared to their methoxy analogs, while the 5-chloro derivative showed a considerable reduction in binding affinity and potency compared to acetyl 2-methoxyisoindolo[2,1-a]indole compound. The 10-methoxy-5,6-dihydroindolo[2,1-a]isoquinolines had higher binding affinities than the corresponding parent indoloisoquinolines in the human receptor subtypes, and the parent compds. were antagonists whereas the 10-methoxy derivs. were agonists in the functional assay. The N-cyclobutanecarbonyl derivs. of both the parent and 10-methoxyl series had similar binding affinities and were both antagonists with similar potencies. The 11-methoxy-6,7-5H-benzo[c]azepino[2,1-a]indoles had higher binding affinities than the corresponding parent compds. at the MT2 receptor but similar affinities at the mtl site; all of the compds. were antagonists in the functional assay. Changing 11-methoxy for 11-ethoxy decreased the binding affinity slightly, and this was more evident at the MT2 receptor. All of the derivs. investigated had either the same or a greater affinity for the human MT2 receptor compared to the mtl receptor (range 1:1-1:132). This suggests that the mtl and MT2 receptor pockets differ in their ability to accommodate alkyl groups in the indole nitrogen region of the melatonin mol. Two compds. were tested in functional assays on recombinant mtl and MT2 melatonin receptors. N-butanoyl 2-(9-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethanamine was a potent

L4 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

agonist with some selectivity (44-fold) for the MT2 receptor, while N-butanoyl 2-(5,6,7-trihydro-11-methoxybenzo[c]cyclohept[2,1-a]indol-13-yl)ethanamine was an MT2-prefering antagonist. Increasing the carbon chain length between N-1 of indole and the 2-Ph group from n = 1 through n = 3 leads to a fairly regular decrease in the binding affinity, but, remarkably, when n = 3, it converts the methoxy compds. from melatonin agonists to antagonists. The Xenopus melatonin receptor thus cannot accommodate an N-n-alkyl chain attached to a 2-Ph substituent with n > 2 in the required orientation to induce or stabilize the active receptor conformation.
 IT 244160-10-9P 263865-08-3P 263865-09-4P 263865-10-7P 263865-11-8P 263865-12-9P 263865-13-0P 263865-14-1P 263865-15-2P 263865-16-3P 263865-17-4P 263865-18-5P 263865-19-6P 263865-20-9P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 derived from isoindoloindoles, indoloisoquinolines, and benzoazepinoindoles)
 RN 244160-10-9 CAPLUS
 CN Butanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (CA INDEX NAME)



RN 263865-08-3 CAPLUS
 CN Acetamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

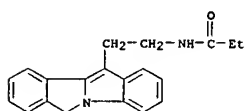


RN 263865-09-4 CAPLUS
 CN Propanamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

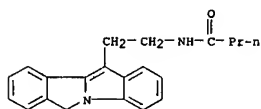
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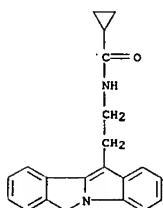
L4 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263865-10-7 CAPLUS
CN Butanamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

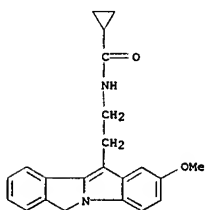


RN 263865-11-8 CAPLUS
CN Cyclopropanecarboxamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

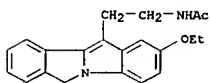


RN 263865-12-9 CAPLUS
CN Cyclobutanecarboxamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

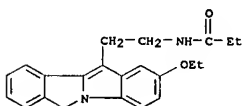
L4 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263865-16-3 CAPLUS
CN Acetamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

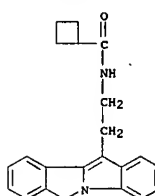


RN 263865-17-4 CAPLUS
CN Propanamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

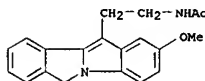


RN 263865-18-5 CAPLUS
CN Butanamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

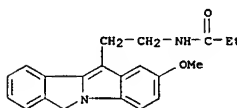
L4 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263865-13-0 CAPLUS
CN Acetamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

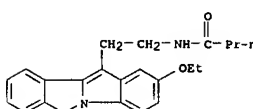


RN 263865-14-1 CAPLUS
CN Propanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

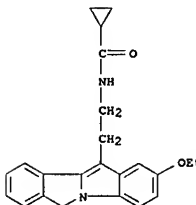


RN 263865-15-2 CAPLUS
CN Cyclopropanecarboxamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

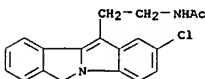
L4 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263865-19-6 CAPLUS
CN Cyclopropanecarboxamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 263865-20-9 CAPLUS
CN Acetamide, N-[2-(2-chloro-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



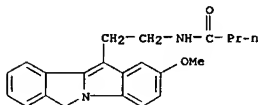
REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

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L4 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:442966 CAPLUS
 DOCUMENT NUMBER: 131:240681
 TITLE: Design of subtype selective melatonin receptor agonists and antagonists
 AUTHOR(S): Sugden, David; Yeh, Li-Kuan; Teh, Muy-Teck
 CORPORATE SOURCE: Physiology Division, GKT School of Biomedical Science,
 SOURCE: King's College London, London, W8 7AH, UK
 Reproduction, Nutrition, Development (1999), 39(3), 335-344
 CODEN: RNDEES; ISSN: 0926-5287
 PUBLISHER: Editions Scientifiques et Medicales Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Studies of the physiol. actions of melatonin have been hindered by the lack of specific, potent and subtype selective agonists and antagonists. We describe the utility of a melanophore cell line from *Xenopus laevis* for exploring structure-activity relationships among novel melatonin analogs and report a novel MT2-selective agonist (I1K7) and MT2-selective receptor antagonist (K185). I1K7 is a potent melatonin receptor agonist in the melanophore model, and in NIH3T3 cells expressing human mtl and MT2 receptor subtypes. In radioligand binding expts. I1K7 is 90-fold selective for the MT2 subtype. K185 is devoid of agonist activity, but acts as a competitive melatonin antagonist in melanophores. A low concentration (10⁻⁹M) antagonizes melatonin inhibition of forskolin stimulation of cAMP in NIH3T3 cells expressing human MT2 receptors, but has no effect in cells expressing mtl receptors. In binding assays, K185 is 140-fold selective for the MT2 subtype.
 IT 244160-10-9
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study) (melatonin analogs structure-activity relationship in frog melanophore and human melatonin receptors)
 RN 244160-10-9 CAPLUS
 CN Butanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (CA INDEX NAME)



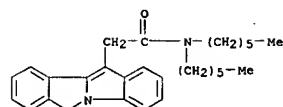
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS

L4 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

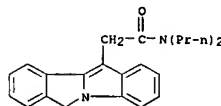
ACCESSION NUMBER: 1993:662000 CAPLUS
 DOCUMENT NUMBER: 119:262000
 TITLE: Chemistry, binding affinities, and behavioral properties of a new class of "antineophobic" mitochondrial DBI receptor complex (mDRC) ligands
 AUTHOR(S): Kozikowski, A. P.; Ma, D.; Brewer, James; Sun, S.; Costa, E.; Romeo, E.; Guidotti, A.
 CORPORATE SOURCE: Mayo Found. Med. Educ. Res., Jacksonville, FL, 32224, USA
 SOURCE: Journal of Medicinal Chemistry (1993), 36(20), 2908-20
 CODEN: JMCMAR; ISSN: 0022-2623
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 119:262000
 AB The mitochondrial DBI (diazepam-binding inhibitor) receptor complex (mDRC; previously called the peripheral benzodiazepine receptors) is linked to the production of neurosteroids such as pregnenolone sulfate, dehydroepiandrosterone sulfate, and others. In order to gain further information as to the function of the mDRC in the brain, the authors have constructed and tested, both in vitro and in vivo, a novel series of ligands, 2-arylindole-3-acetamides. The SAR studies detailed herein delineate some of the structural features required for high affinity binding to the mDRCs. In most cases the new ligands were prepared by use of the Fischer indole synthesis. Variations in the length and number of the alkyl groups on the amide nitrogen were probed together with the effects of halogen substituents on one or both of the aryl rings. Some ligands were also synthesized for study which represent conformationally constrained versions of the parent structure. Broad screening studies revealed these indoleacetamides to be highly selective for the mDRC, since they failed to bind with any significant affinity to other receptor systems. Some of the ligands were found to exhibit Ki values in the low nanomolar range for the mDRC as measured by the displacement of [3H]4'-chlorodiazepam. A subset of these ligands was also shown to stimulate pregnenolone formation from the mitochondria of C6-2B glioma cells with an EC50 of about 3 nM. In animal expts. ligands selected for further study were found to exhibit antineophobic effects, in spite of the fact that they exhibit no direct action on GABAA receptors. Consequently, it is postulated that these ligands owe their action to an indirect modulation of GABAA receptor function, presumably by stimulation of neurosteroid production and release from glial cells, followed by neurosteroid modulation of GABA's action on the chloride ion channel conductance of GABAA receptors.
 IT 147375-21-1P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and mitochondrial diazepam-binding receptor complex affinity of, glial neurosteroid release and GABAA receptor function modulation and antineophobic activity in relation to)
 RN 147375-21-1 CAPLUS
 CN 6H-Indolo[2,1-a]indole-11-acetamide, N,N-dihexyl- (9CI) (CA INDEX NAME)

L4 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
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L4 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 135966-96-0P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and mitochondrial diazepam-binding receptor complex affinity of, glial neurosteroid release and GABAA receptor function modulation in relation to)
 RN 135966-96-0 CAPLUS
 CN 6H-Indolo[2,1-a]indole-11-acetamide, N,N-dipropyl- (9CI) (CA INDEX NAME)



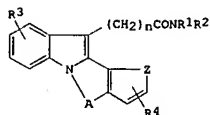
11/06/2007

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L4 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1993:233880 CAPLUS
 DOCUMENT NUMBER: 118:233880
 TITLE: Preparation of indolecarboxamides and methods of treating neurological and psychiatric disorders
 INVENTOR(S): Costa, Erminio; Guidotti, Alessandro; Kozikowski, Alan; Ma, Dawei
 PATENT ASSIGNEE(S): Fidia - Georgetown Institute for the Neurosciences, USA
 SOURCE: PCT Int. Appl., 55 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9300334	A1	19930107	WO 1992-US5246	19920626
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
US 5206382	A	19930427	US 1991-722196	19910627
AU 9222939	A	19930125	AU 1992-22939	19920626
EP 546164	A1	19930616	EP 1992-914902	19920626
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
JP 06501030	T	19940127	JP 1993-501593	19920626
US 1991-722196 A 19910627				
WO 1992-US5246 A 19920626				

PRIORITY APPLN. INFO.:
 OTHER SOURCE(S): MARPAT 118:233880
 GI



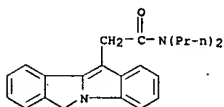
AB Title compds. I (R1, R2 = H, C3-12 alkyl, (alkyl)aryl; R1R2 = 4-6-membered (un)saturated ring; R3, R4 = H, C1-12 alkyl, O2N, H2N, N3, cyano, halo, RO2C, RO, RS (wherein R = H, alkyl); A = C1-3 alkylene to form a ring or null; Z = O, NH, S, CH:CH; n = 1-3) or their salts are prepared PhNHNH2, PhCOCH2CH2CO2H and H2SO4 in EtOH were refluxed for 24 h, cooled and extracted

L4 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1991:535868 CAPLUS
 DOCUMENT NUMBER: 115:135868
 TITLE: Palladium catalyzed synthesis of annelated indoles
 AUTHOR(S): Kozikowski, Alan P.; Ma, Dawei
 CORPORATE SOURCE: Mayo Clin., Jacksonville, FL, 32224, USA
 SOURCE: Tetrahedron Letters (1991), 32(28), 3317-20
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 115:135868
 GI

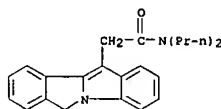
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The synthesis of polycyclic indoles, e.g., I (X = O, CH2), II, III, is shown to be accomplished readily by the palladium catalyzed intramol. cyclization of bromoarylindoles, e.g., IV, V, VI.

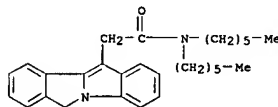
IT 135966-96-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 135966-96-0 CAPLUS
 CN 6H-isoindolo[2,1-a]indole-11-acetamide, N,N-dipropyl- (9CI) (CA INDEX NAME)



L4 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 with Et2O to give Et 2-phenyl-3-indoleacetate which in 3N NaOH was refluxed for 3 h, acidified with HCl and treated with Me(CH2)5NH2, PhOP(O)(Cl)NHPh, and Et3N to give I (A = null, Z = CH:CH, R1 = R3 = H, R2 = hexyl, n = 1). I showed anxiolytic action in rodents at 0.1-0.5 mg/kg.
 IT 135966-96-0P 147375-21-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as drug for treatment of neurol. disorders and as antipsychotics)
 RN 135966-96-0 CAPLUS
 CN 6H-isoindolo[2,1-a]indole-11-acetamide, N,N-dipropyl- (9CI) (CA INDEX NAME)



RN 147375-21-1 CAPLUS
 CN 6H-isoindolo[2,1-a]indole-11-acetamide, N,N-diethyl- (9CI) (CA INDEX NAME)



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LOGOFF? (Y)/N/HOLD:Y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

63.71

236.02

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

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-9.36

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